The Use of Computational Chemistry to Obtain Thermodynamic Information for Problems of Environmental Interest (Invited)

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In recent years there have been major advances in the accuracy and ease of use of computational quantum chemistry programs, though so far these have had little impact on chemical engineering practice. Here we will show how the information obtained from such programs can be used to provide accurate predictions of octanol-water partition coefficients and Henry's law (air-water partition) coefficients, and how such information can be used for estimating the fate of chemicals released to the environment. Also, we will discuss how quantum chemistry calculations can be used to remove some of the failings of group contribution methods.